1,2,3-Trichloropropene
96-19-5 | DTXSID3047766

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 5.42 days

Global applicability domain: Inside

Local applicability domain index: 5.69e-01

Confidence level: 7.81e-01

Nearest Neighbors from the Training Set

Image not found
Isobutylbenzene
Measured: 201
Predicted: 6.97

Image not found
1,3-Diethylbenzene
Measured: 88.3
Predicted: 5.36

Image not found
1,3-Dimethylcyclopentane
Measured: 24.3
Predicted: 4.08

Image not found
1,3-Dimethyl-5-ethylbenzene
Measured: 4.93
Predicted: 3.64

Image not found
Ethylbenzene
Measured: 120
Predicted: 6.21